Depuis 80 ans, nos connaissances bâtissent de nouveaux mondes

Apprentissage automatique en chimie et en science des matériaux

Jean-Claude Crivello, ICMPE
crivello@icmpe.cnrs.fr

Le «*AI boom*»

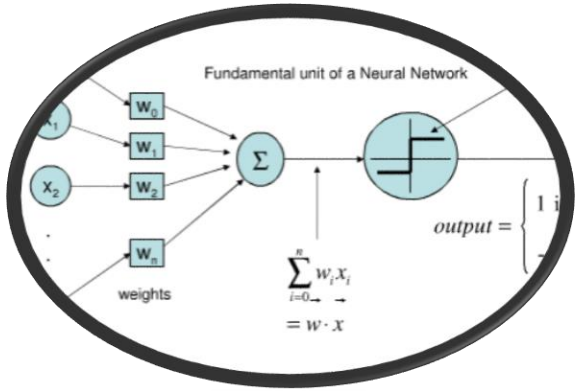
1950

Turing test

1956

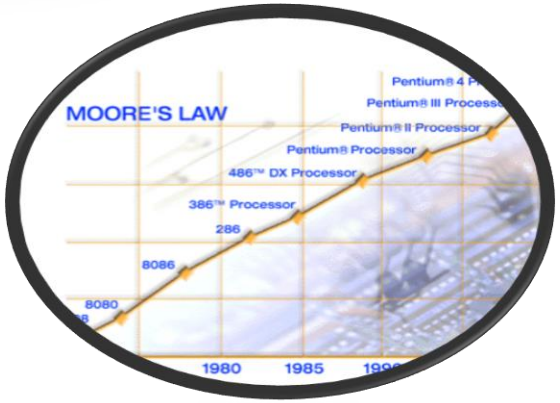
« *artificial intelligence* »

1969



Minsky: *Perceptron*

1975

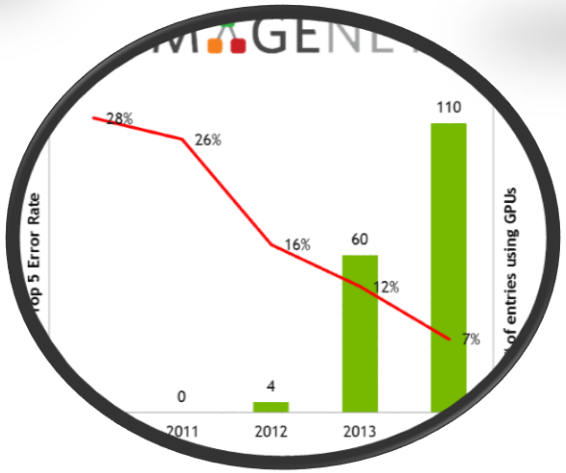


Moore’s law

1990

Convolutional Neural Networks

2012



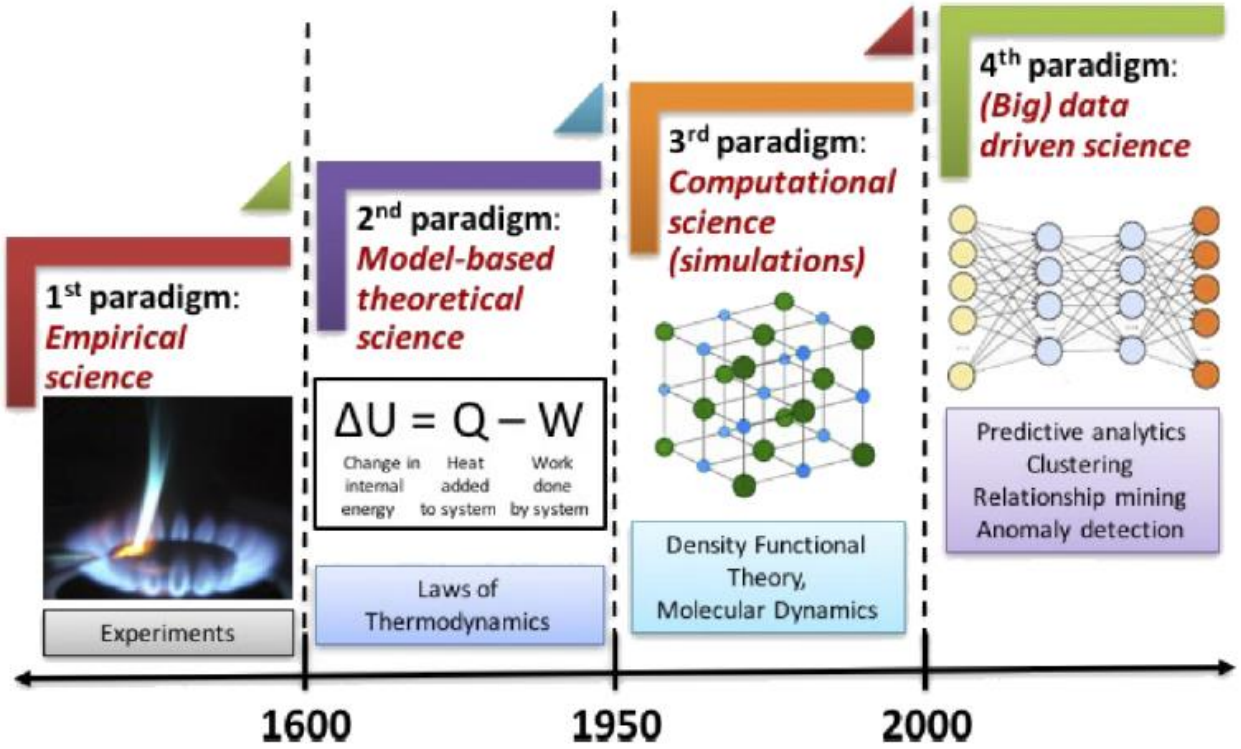
Imagenet Challenge

now

IA: vers un nouvel paradigme en chimie ?

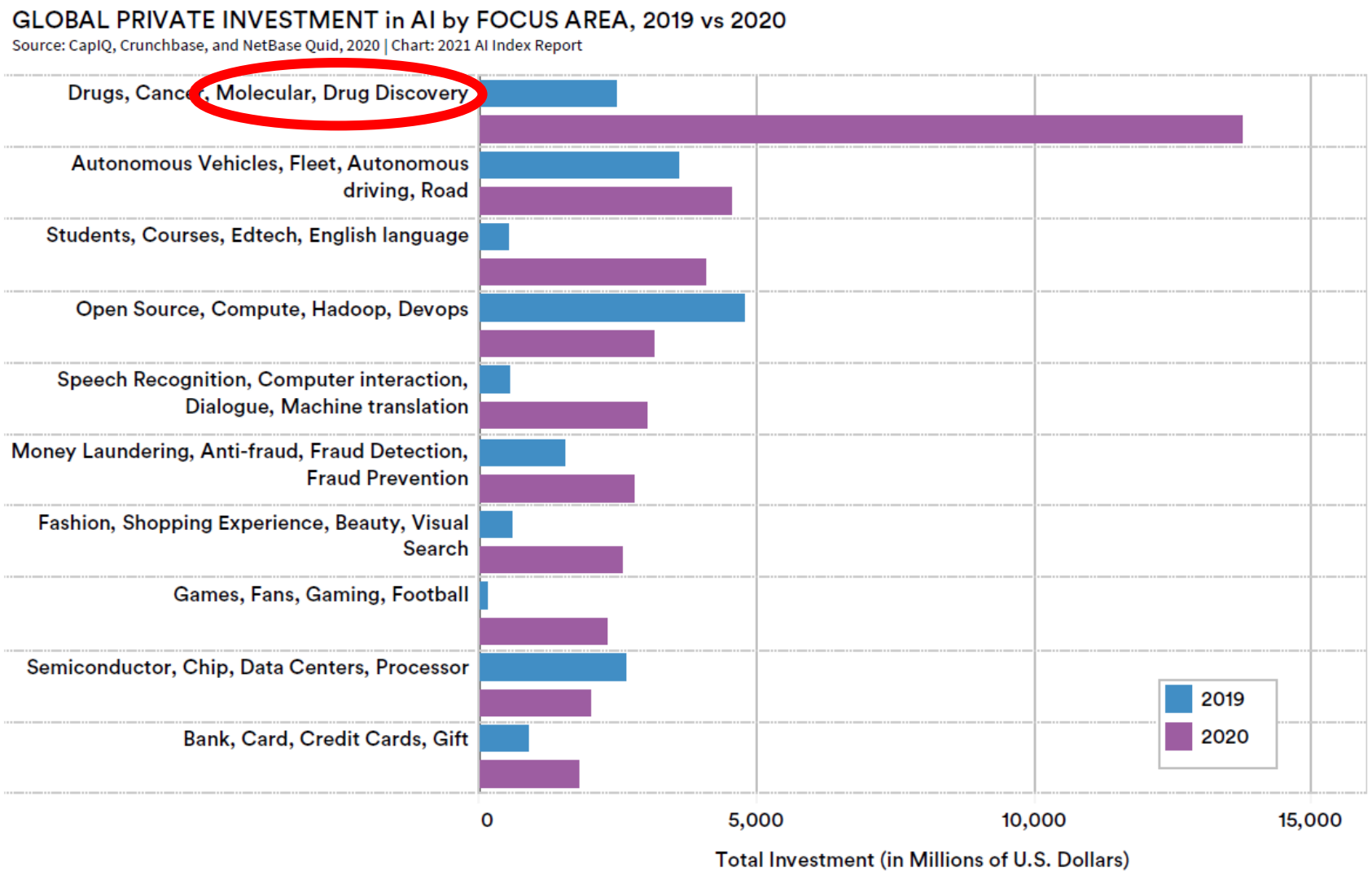
TMS2019: « Computational Approaches for Big Data, Artificial Intelligence, machine learning »

Agrawal *et al*.
Perspective: Materials informatics and big data: realization of the « fourth paradigm » of science in materials science
APL Materials (2016)



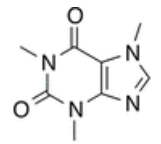
Disciplines privilégiées en 2020

Artificial Intelligence Index Report 2021



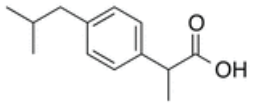
Découverte de nouvelles molécules

- Représentation textuelle SMILE
- Algorithmes dédiés au texte (NPL, GPT)
- Théorie des graphes



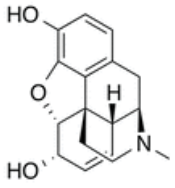
Caffeine

CN1c2ncn(C)c2C(=O)N(C)C1=O



Ibuprofen

CC(C)Cc1ccc(cc1)C(C)C(O)=O



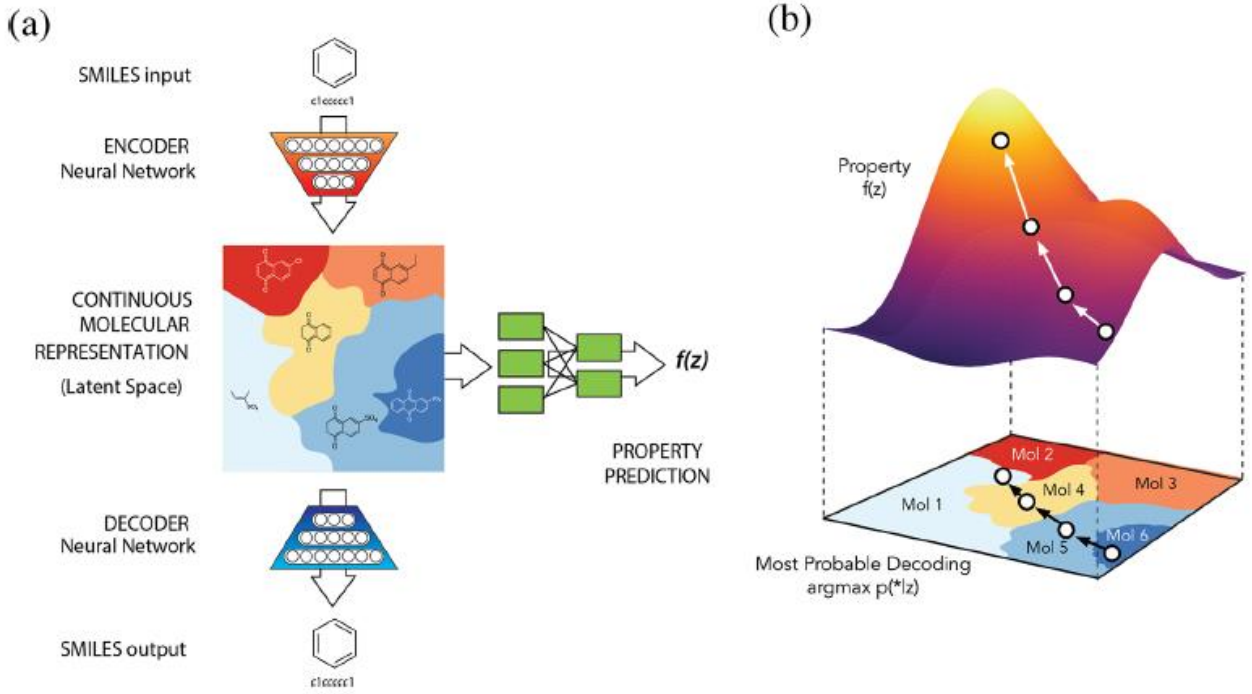
Morphine

[H][C@]12C=C[C@H](O)[C@@H]3Oc4c5c(C[C@H]1N(C)CC[C@@]235)ccc4O

Batch	Generated Example	valid
0	Oc.BK5i%ur+7oAFc7L3T=F8B5e=n)CS6RCTAR((OVCp1CApb)	no
1000	OF=CCC2OCCCC)C2)C1CNC2CCCCCCCCCCCCCCCCCCCCCCC	no
2000	O=C(N)C(=O)N(c1occc1OC)c2ccccc2OC	yes
3000	O=C1C=2N(c3cc(ccc3OC2CCC1)CCCc4cn(c5c(Cl)cccc54)C)C	yes

Segler *et al*. ACS central science (2018)

Generating Focused Molecule Libraries for Drug Discovery with Recurrent Neural Networks

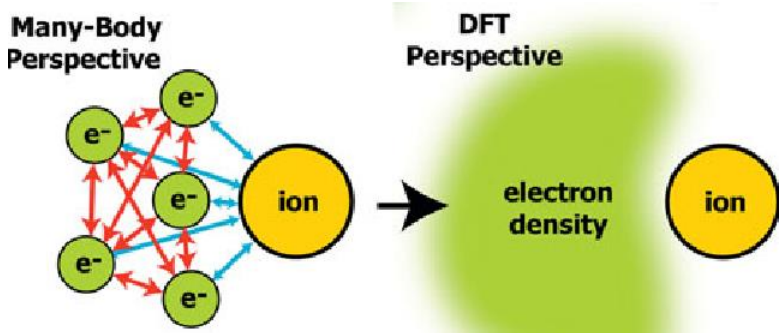


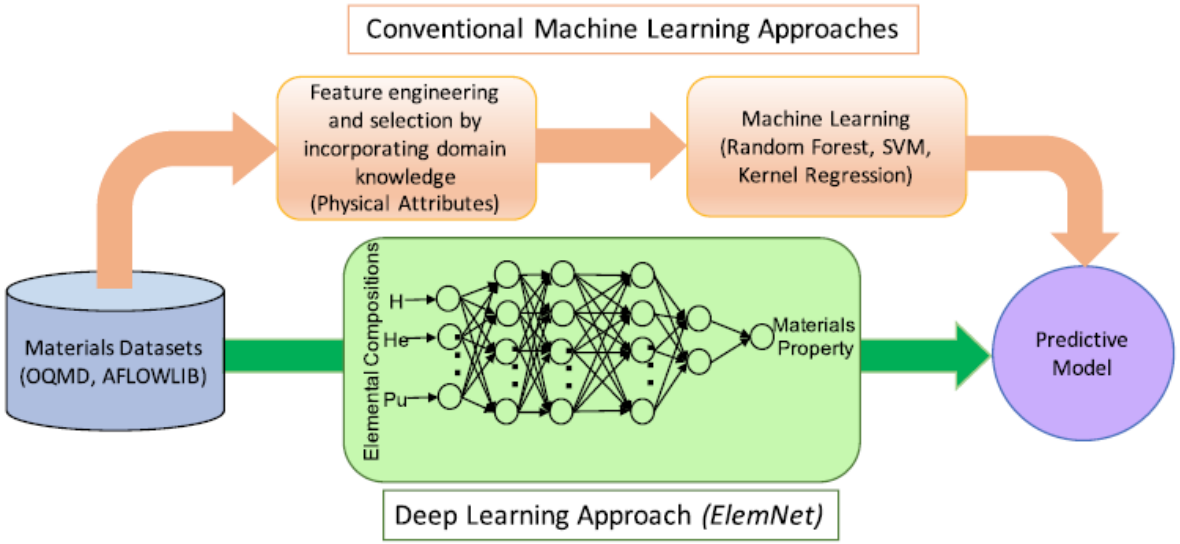
Gomez-Bombarelli *et al*. ACS central science (2018)

Automatic Chemical Design Using a Data-Driven Continuous Representation of Molecules

Du *Materials Genome Initiative* au *Machine Learning*

N. Nosenko. Nature (2016)
The material code





Jha, Wolverton, Agrawal *et al*. Scientific report (2018)
ElemNet: Deep Learning the Chemistry of Materials From Only Elemental Composition

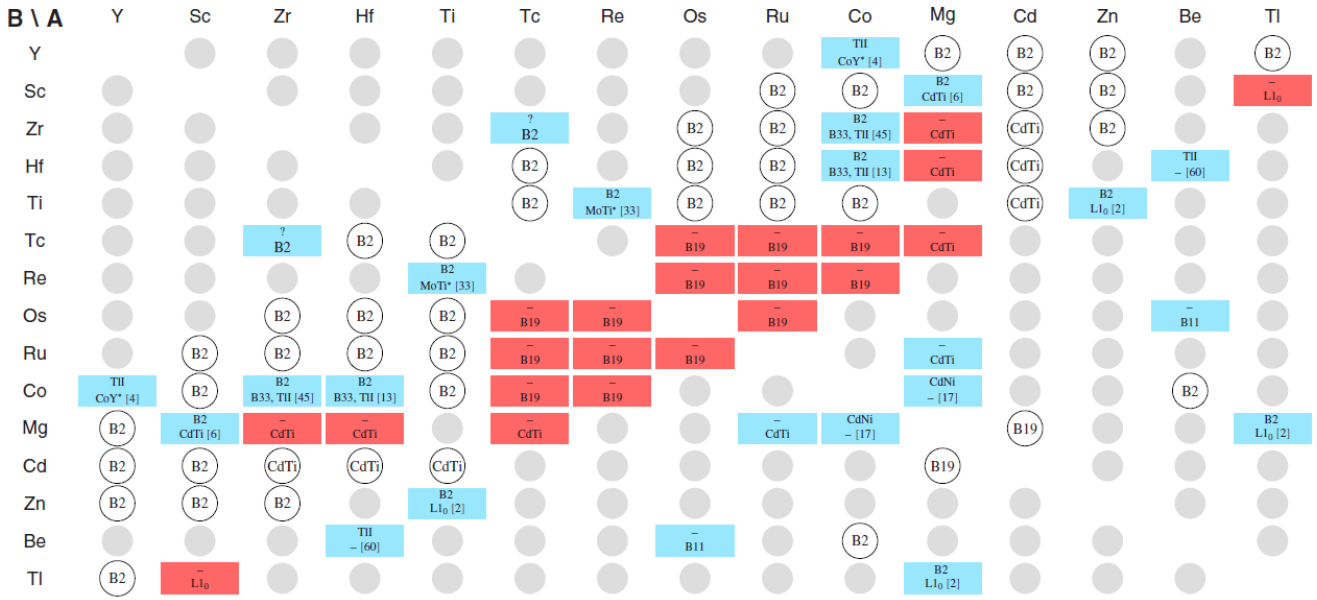
Exemples d’applications de l’IA en chimie

- Data-mining algorithms

  High-throughput screening, combinatory analyze, …

Levy, Hart, Curtarolo.
Phy Rev B (2010)
Structure maps for hcp metals from first-principles calculations

http://aflowlib.org/

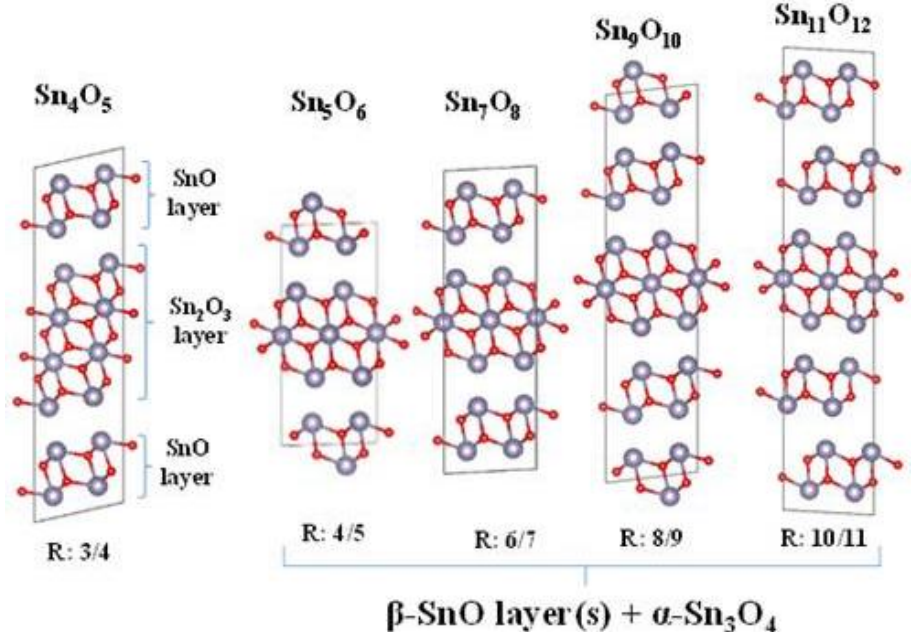


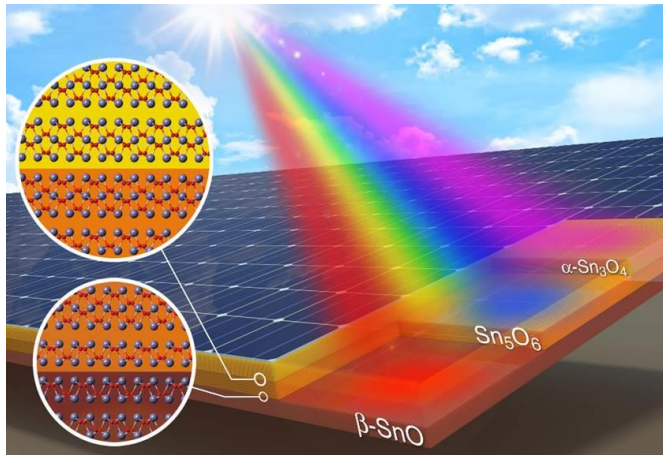
Exemples d'applications de l'IA en chimie

- Data-mining algorithms
- Optimization algorithms

  Genetic algorithm, Evolutionary methods …

Wang, Umezawa, Hosono. Advanced Energy Materials (2016)
Mixed Valence Tin Oxides as Novel van der Waals Materials.

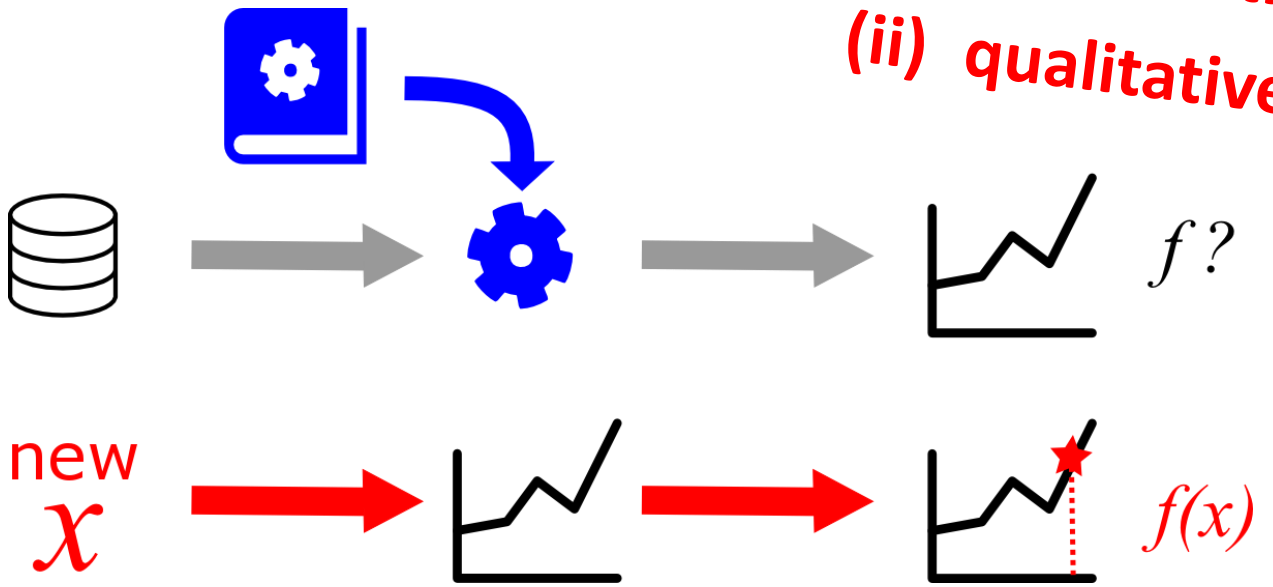




Exemples d'applications de l'IA en chimie

- Data-mining algorithms
- Optimization algorithms
- Machine learning algorithms (ML)
  - Unsupervised learning (*clustering*)
  - Reinforcement learning
  - Supervised learning

(i) quantitative or
(ii) qualitative variables?

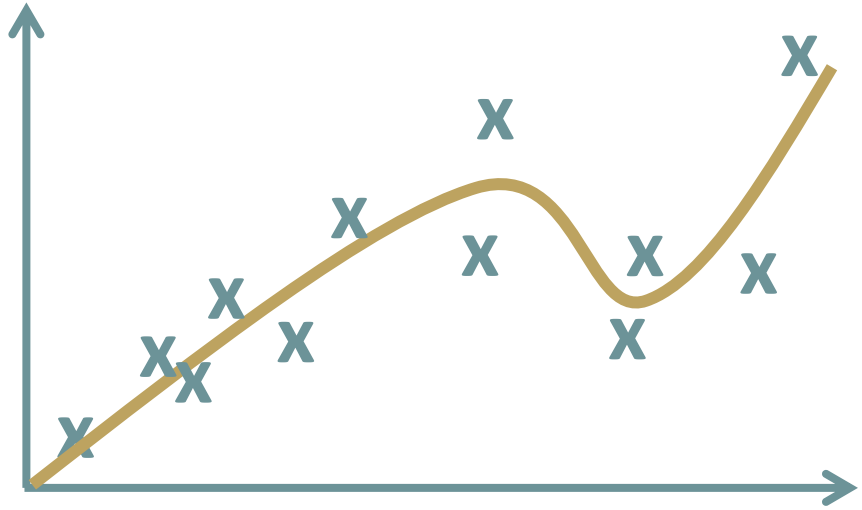


Exemples d'applications de l'IA en chimie

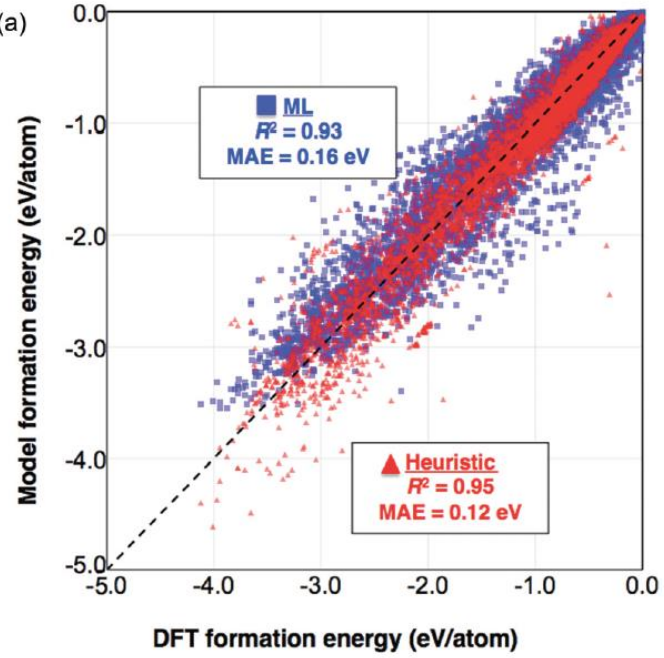
(i) Quantitative variable

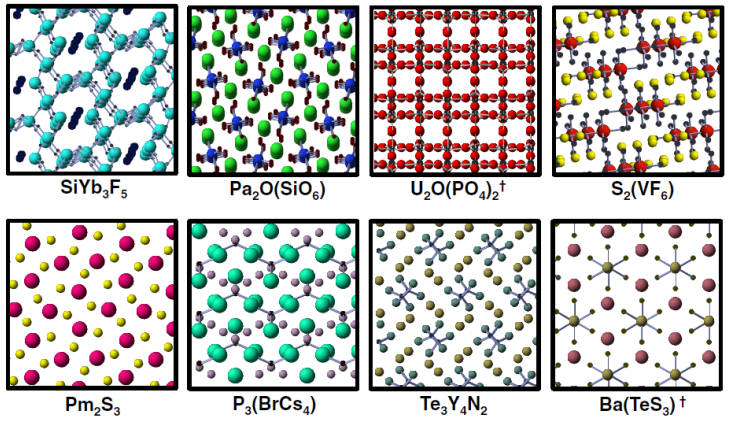
→ **Regression algorithms**

- Linear, non-linear



Meredig, Wolverton *et al*.
Phy Rev B (2014)
Combinatorial screening for new materials in unconstrained composition space with machine learning



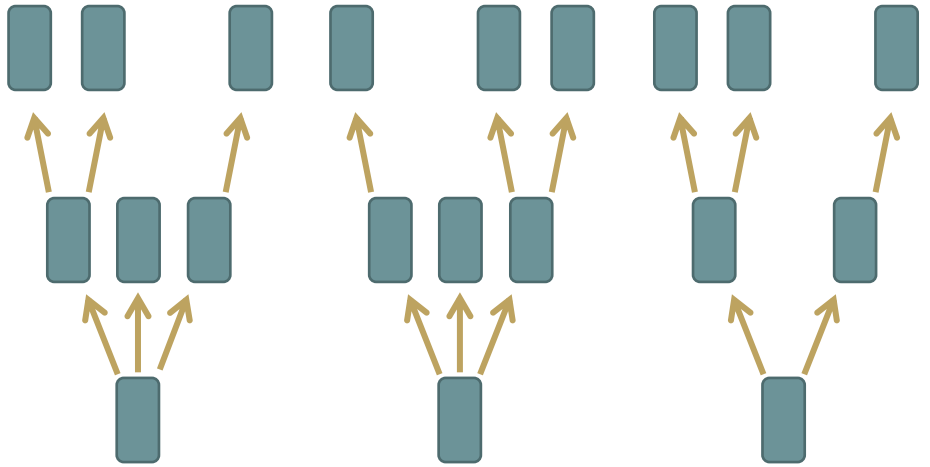


Exemples d'applications de l'IA en chimie

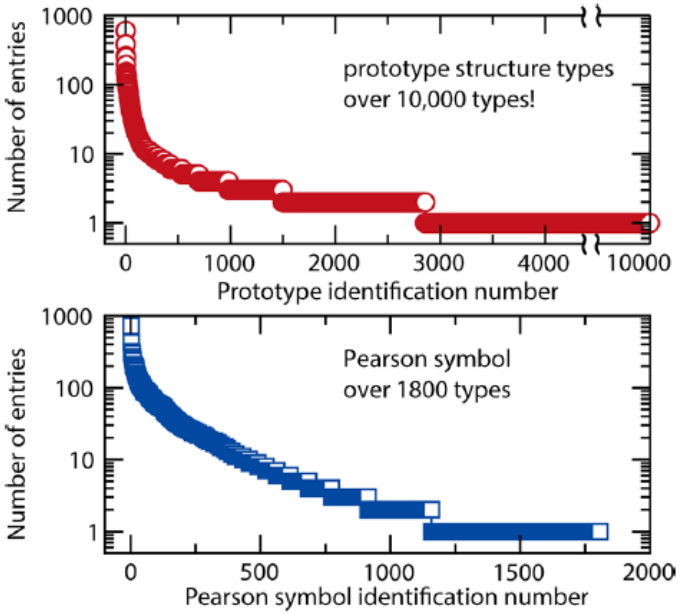
(ii) Qualitative variable

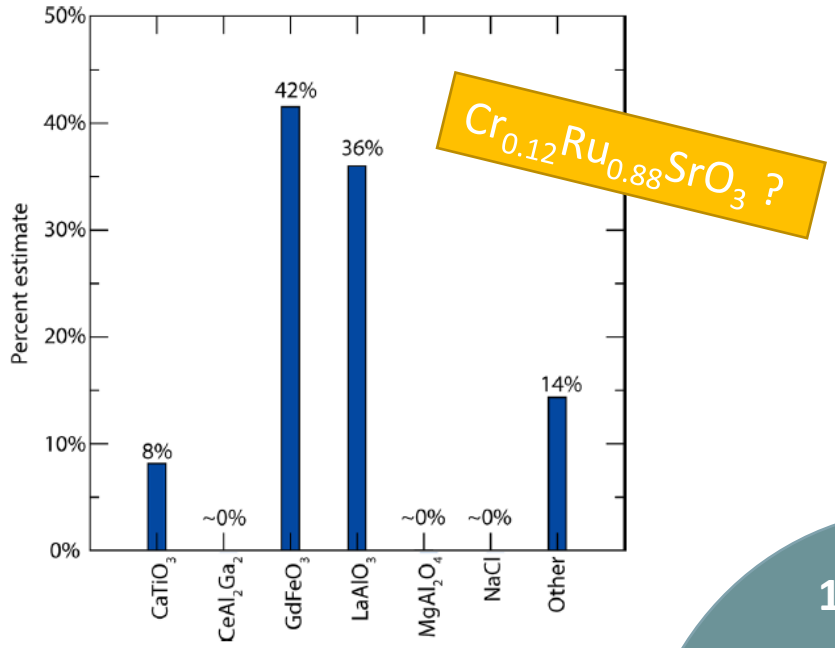
→ **Classification algorithms**

- Decision tree, **random forests**



Graser, Sparks *et al*.
Chem Mater (2018)
Machine Learning and Energy Minimization Approaches for Crystal Structure Predictions: A Review and New Horizons

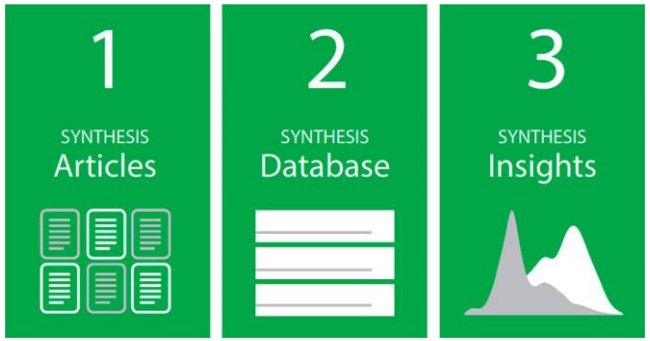


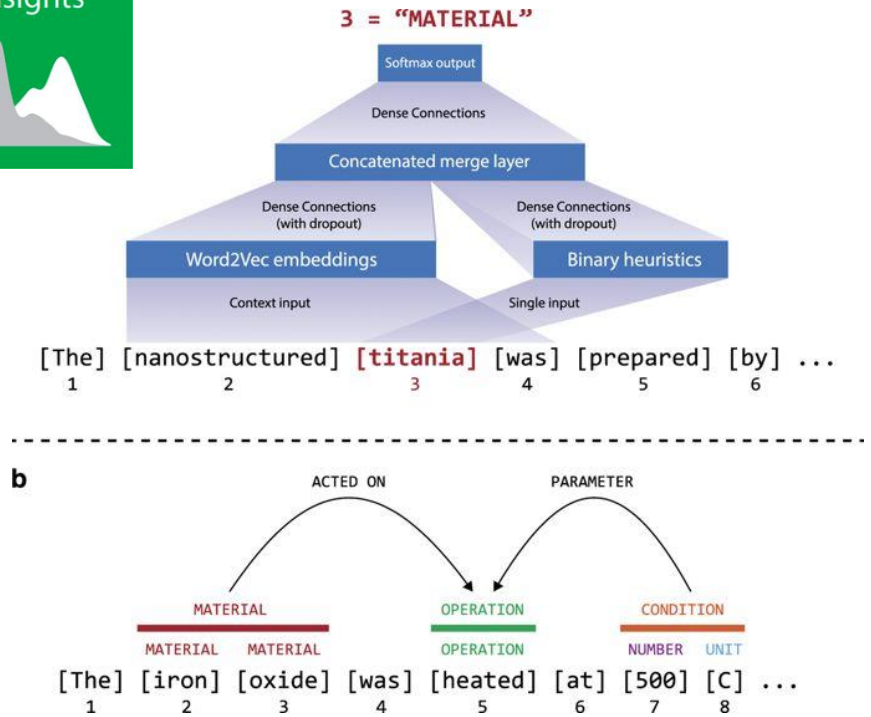


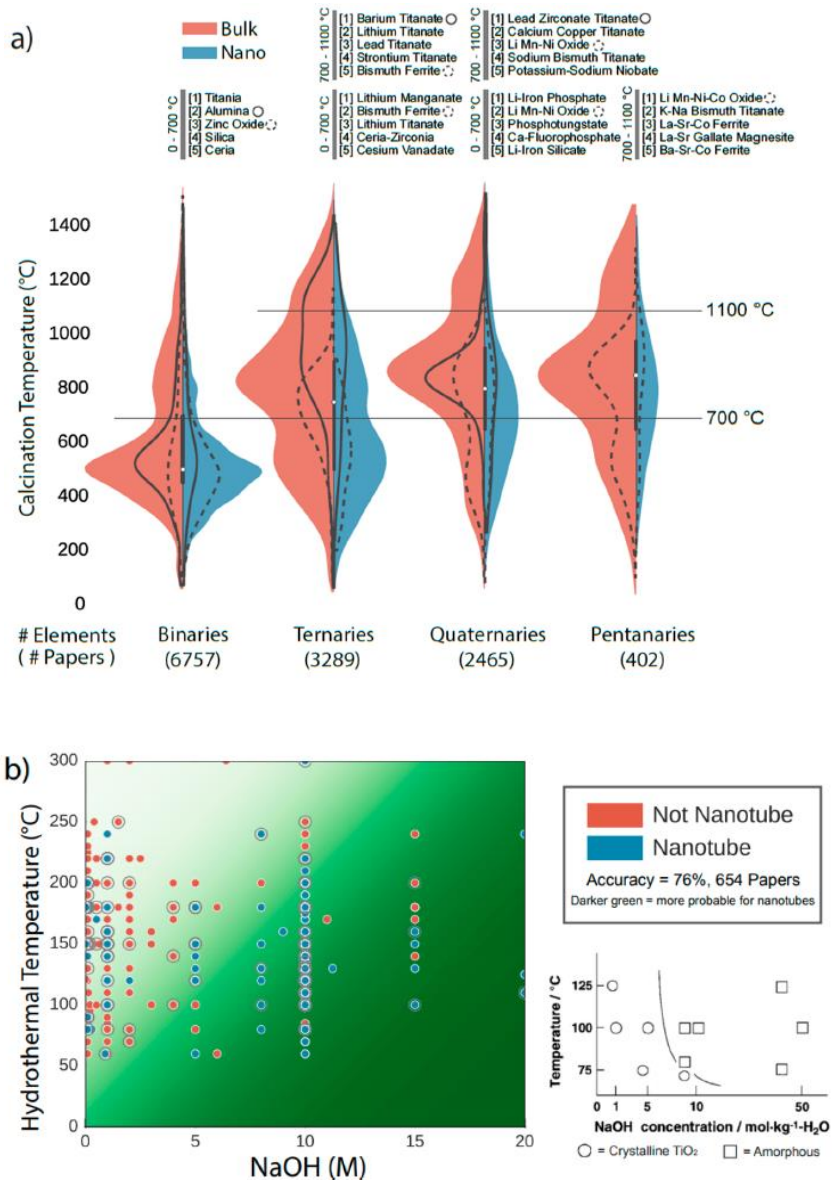
Global methods

Kim, Saunders, Ceder, Olivetti *et al*. Chemistry of materials (2017)

Materials synthesis insights from scientific literature via text extraction and machine learning

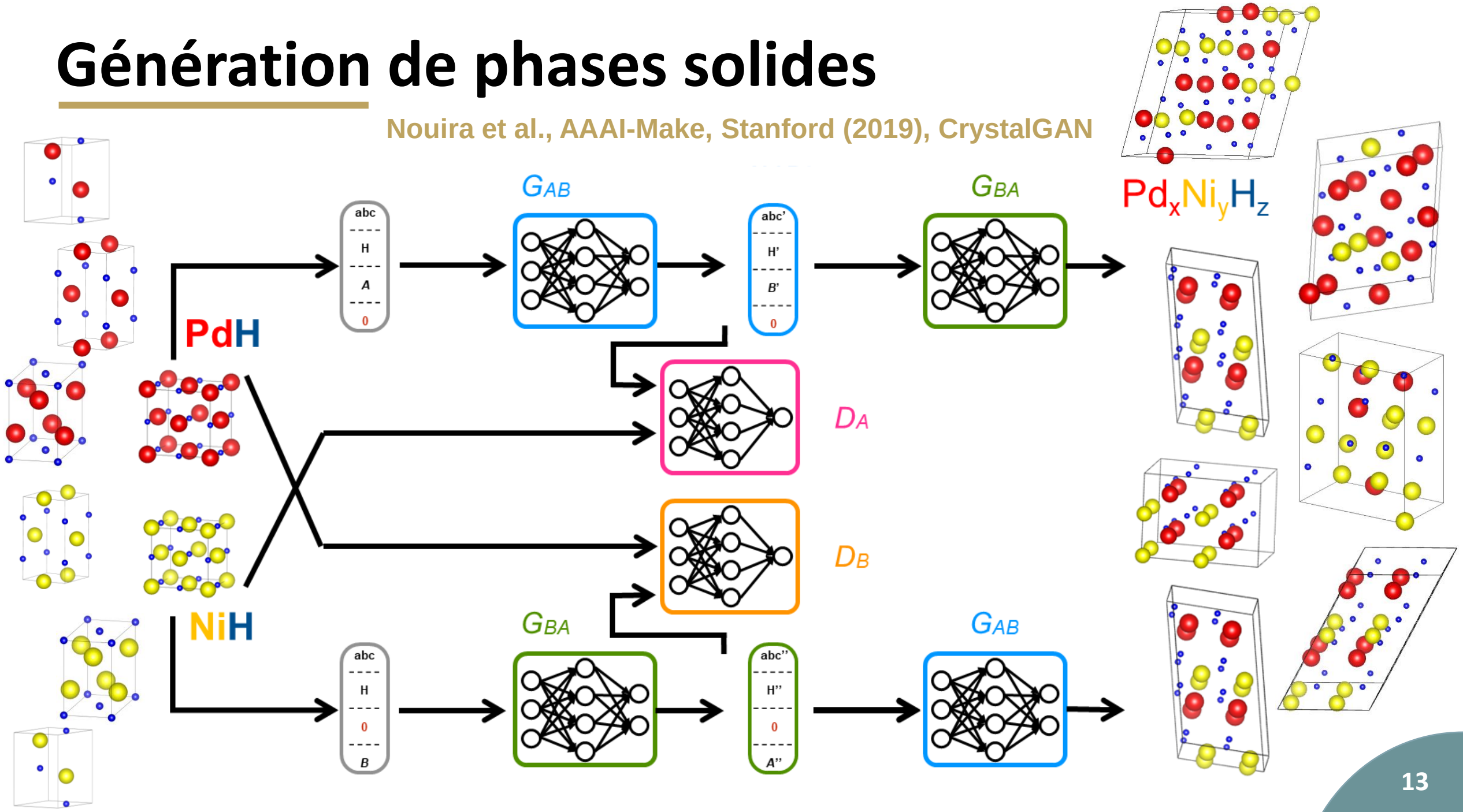




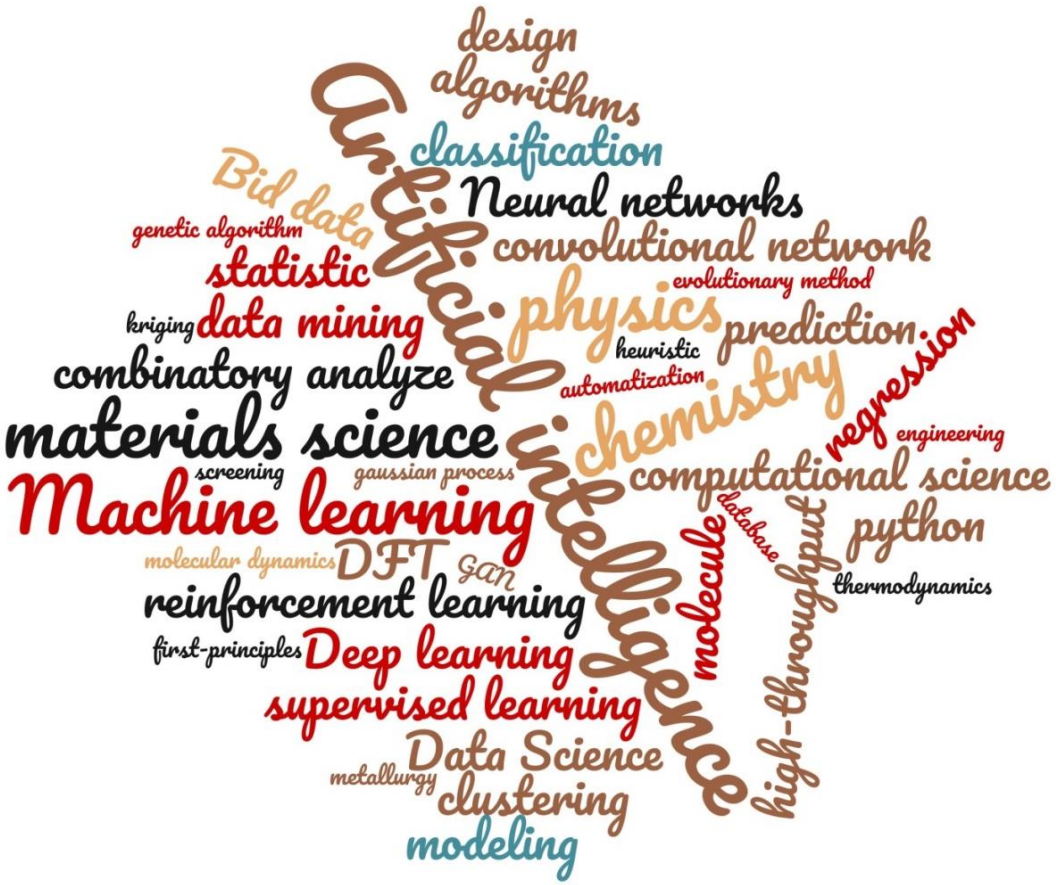


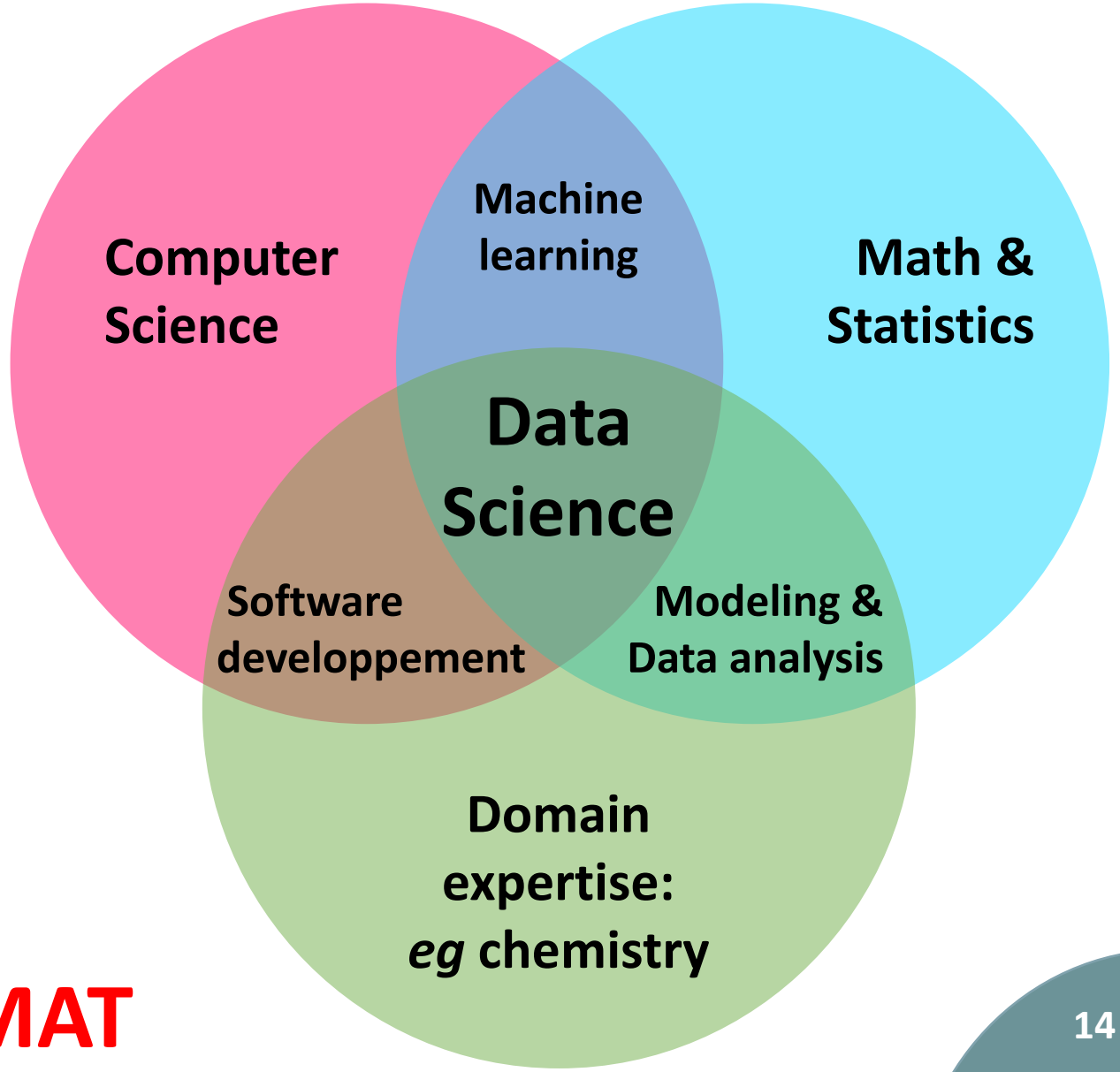
Génération de phases solides

Nouira et al., AAAI-Make, Stanford (2019), CrystalGAN



L'IA : une science interdisciplinaire





→ **Création d'un GDR IAMAT**